Analysis of Stress due to Biomolecular Adhesion on Cantilever Surface

An Integrated Optic Approach

Malathi Sathish*, Srinivas Talabattula

Applied Photonics Lab, Dept of ECE, Indian Institute of Science, Bangalore, India

* sathishvac@gmail.com

Abstract

In this work, we have designed, optimized an integrated optic biosensor by analytical method and numerical simulations. The device consists of a racetrack resonator and a cantilever on silicon on insulator wafer. We proved its ability to distinguish tensile and compressive stress developed during conformation of protein molecules on the cantilever surface. By FDTD simulations, we observed that resonant wavelength shifts by +1.56 nm (red shift) with a compressive strain of -15000 με and -1.6 nm (blue shift) with a tensile strain of +15000 με.

Keywords

Biosensor; Cantilever; Conformation; Integrated Optic; Protein; Resonator; Silicon on Insulator

Introduction

Physical, Chemical and Biological sensors have been reported with micro-fabricated cantilever structures that are extremely sensitive. With vast developments in the field of MEMS and in particular first demonstration of Atomic Force Microscopy (AFM) for biosensing applications have opened a new avenue in biosensing [Marti et al.,]. These cantilever structures enable us to monitor adsorption of Proteins whose structure undergoes conformational changes during incubation period.

Normally the cantilevers are operated in static mode for bio applications while working in liquid environment. If the structures are operated in dynamic mode, damping due bio fluid would strongly influence the resonant characteristics. Optical lever detection scheme is well known technique to extract information from the sensor. But the laser beam undergoes scattering while passing through the turbid medium, also the total optical path length is ~ 1m which hinders miniaturization of biosensors.

In this work, we propose an Integrated Optic (IO) racetrack resonator based sensor. The light passes through the waveguide structure by total internal reflection, hence completely decoupled from liquid environment.

Theory

Biomolecules adhere on the functionalized cantilever surface and depending on the type of surface stress the beam bends. In this study we have considered Bovine Serum Albumin (BSA) -which exerts a tensile stress on cantilever bends it upward, where as stress produced by Immuno Globulin G (IgG) is compressive and bends the beam downward. We prove in this work, the ability of the sensor to distinguish tensile and compressive stresses.

Racetrack resonator (RTR) is a unique structure with a microring resonator and a directional coupler. The schematic diagram of a RTR with an arm on the fixed end of a silica cantilever over which proteins would be attached is shown in fig.1. Symbols 't' and 'k' in the diagram represents transmission and coupling coefficients respectively. This configuration is referred as an all pass resonator which has a single bus waveguide to couple light into and out of the resonator. This architecture has the following advantages:

- Good control over coupling coefficient
- Easy integration with mechanical structures

Resonators under critical coupling (power transferred from bus waveguide into ring would be equal to the losses), through port output is completely zero. Under this condition, spectral response of the resonator is steep hence posses high-Q factor and sensitivity.

When biomolecules adhere to the surface of the cantilever it bends either upward or downward. At the fixed end of the cantilever maximum stress develops which is transferred to the Silicon strip waveguide on top and changes the effective index of the propagating mode. This phenomenon is referred as Photo-Elastic

effect or Opto- Mechanical coupling.

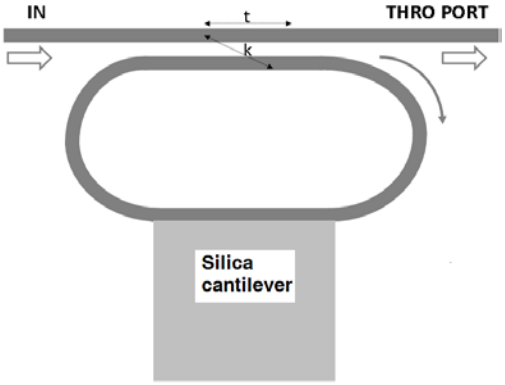

FIG. 1 SCHEMATIC DIAGRAM OF THE SENSOR WITH RACETRACK RESONATOR AND CANTILEVER

In our earlier work, we reported a rib waveguide RTR on Silicon On Insulator (SOI), whose bend radii are normally few 100 μm [Malathi et al.,]. A strip waveguide facilitates us to design and fabricate RTR with ring radii down to few microns. The following sections explain waveguide design, cantilever design, resonator design by analytical and numerical methods.

Waveguide design

The top device layer on the chosen SOI wafer is 1 μm, with a buffer of silica of thickness 1μm on Silicon substrate.

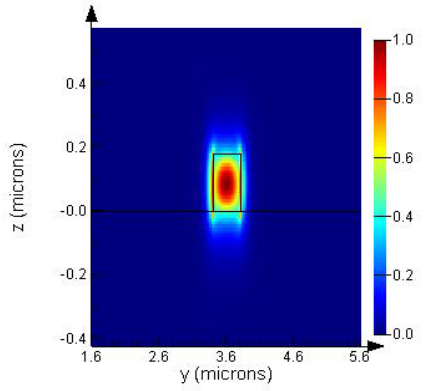

FIG. 2 MODE PROFILE OF A FUNDAMENTAL QUASI-TE MODE

The waveguide dimensions are optimized as shown below:

Width 400nm

Height 180nm

We simulated the device using a simulation tool Eigen mode solver ™ which considers the dispersion due to high index contrast of SOI material [Klein et al.,]. The mode field profile of Quasi-TE0 mode in the strip waveguide is shown in fig.2.

Cantilever Design

The buffer (Silica) layer is extended as the cantilever, on the fixed end of the beam, one arm of the RTR rests. In this work, we assume mechanical properties of silicon and silica micro-structures are elastic in nature; the deformed structure regains its original shape when the applied external forces are removed [Bao et al.,]. The cantilever parameters are:

- L- Length
- W- width
- h- Height (Thickness)

Vibration frequency of the cantilever is given by eq.1.

$$\omega_1 = 1.019 \frac{h}{L^2}\sqrt{\frac{E}{\rho}} \quad (1)$$

where ω_1 - natural frequency of vibration

E- Young's modulus

ρ - density

For bio sensing applications the natural frequency of the cantilever should be larger than 5 KHz [Eriksen et al.,]. Hence we have analysed the vibration frequency of the beam and plotted in fig.3 as a function of buffer thickness. Our simulations revealed buffer thickness of 1 μm has lowest substrate leakage loss, hence 100 μm length beam having vibration frequency around 15 KHz is chosen for as a biosensor. To optimize the beam width, we need to design the racetrack parallel arm (coupler - region) which is presented in the following section.

Racetrack Resonator Design

We aim at miniaturizing the device for Lab-on-Chip applications, hence chosen the radius of resonator as 3μm.

Coupler parameters:

- L_{para} - Parallel length
- L_{cross} - Cross over length
- $L_{critical}$ - power coupled is equal to losses in resonator
- g- Gap between waveguides
- β_e , β_o - propagation constants of even and odd mode
- κ - coupling /length
- K - Power coupling coefficient

Coupling length (L_{cross}) at which power is completely transferred from one waveguide to another of a co-directional coupler can be calculated from propagation constants of supermodes as shown in eq.2. Coupling per unit length and power coupling coefficient are estimated [http://www.photonics.umd.edu/software/wgmodes] with expressions given in eq.3 and eq.4.

$$L_{cross} = \frac{\pi}{2(\beta_e - \beta_o)} \quad (2)$$

$$\kappa = \frac{\pi}{2L_{cross}} \quad (3)$$

$$K = \sin^2(\kappa L_{critical}) \quad (4)$$

With L_{para} values varying from 10 μm to 50 μm in steps of 10 μm, we calculated critical coupling length for different gaps . The simulations reveal for smaller gaps 100nm to 300nm the critical coupling lengths do not vary much.

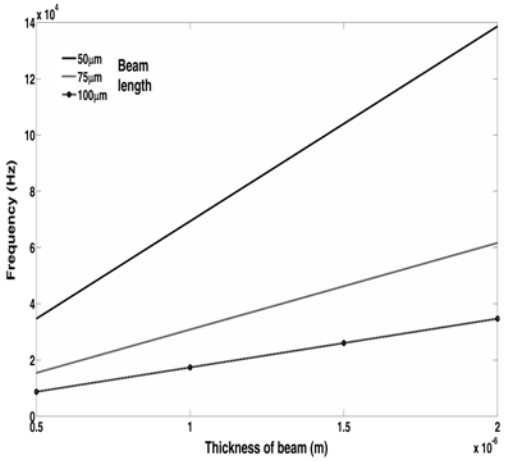

FIG.3 VIBRATION FREQUENCY OF A CANTILEVER

Real field components of the super mode propagating in the coupler section is shown in fig.4. In each colour line represents equal value, and has a step of -3dB , with minimum (outer line) as -39 dB [Rouger et al.,].

If width of the cantilever is too low, surface available for immobilization would be low and affect the uniformity of biomolecules. On the other hand, if we choose a wider beam, the process of etching would take longer duration impacting the process yield [Joshi et al.,]. Hence we fixed the parallel arm length (width of cantilever) as 10μm.

Opto Mechanical Coupling

We assume in this analysis, surface stress on cantilever

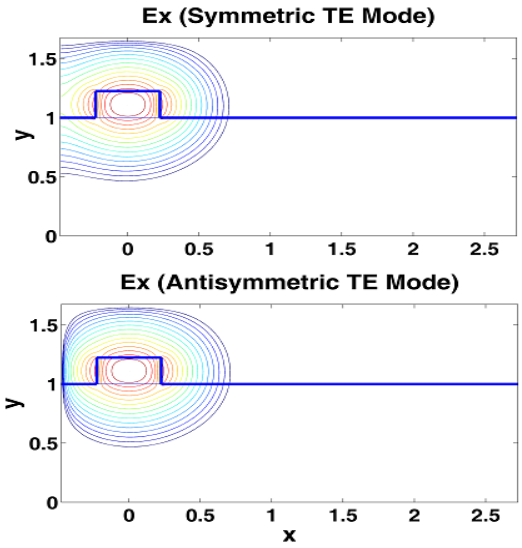

FIG.4 REAL FIELD COMPONENTS OF SYMMETRIC AND ANTISYMMETRIC SUPERMODE WITH A GAP OF 500NM

is uniform and silicon waveguide experiences same level of stress as that of the beam. Pockel [Carpenter et al.,] proposed a theory of photo-elasticity and quantified refractive index when an optical element encounters stress/strain.

Change in the index of refraction [Bhola at al.,] 'n' with applied strain 'ε' for TE polarization is given by eq.5.

$$\frac{\Delta n}{n} = -\frac{n^2 \varepsilon}{2}\left[P_{12} - \nu\left(P_{11} - P_{12}\right)\right] \quad (5)$$

where P_{11} and P_{12} are stress -optic coefficients.

We consider the strain in the range between +15000 με and -15000 με: where positive sign indicates Tensile and negative sign indicates Compressive strain. Analytically we found that tensile stress blue shifts the resonant wavelength where as compressive stress red shifts the resonance. The simulation results are shown in fig.5.

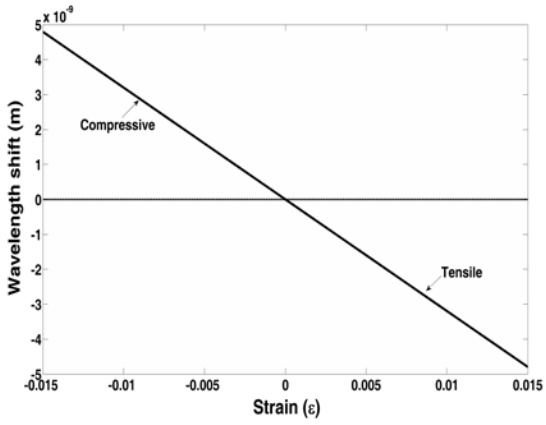

FIG.5 RESONANT WAVELENGTH SHIFT FOR COMPRESSIVE AND TENSILE STRAINS

The resonant wavelength undergoes +4.794 nm shifts with -15000 με and -4.794 nm for +15000 με strain values.

FDTD Lumerical™ based numerical simulations are carried out for the same set of strain values with a layout shown in fig.6.

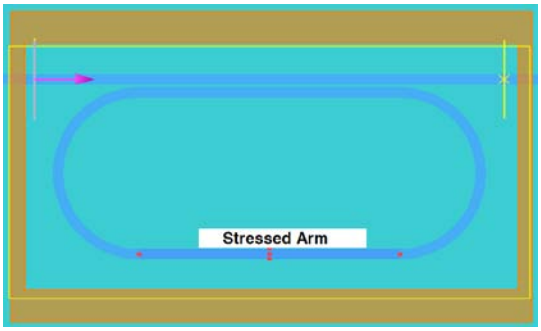

FIG. 6 FDTD LAYOUT OF STRESSED RACETRACK RESONATOR

The racetrack has a radius of 3μm (curved section) and straight waveguides of 10μm length. One of the parallel waveguides couples light into and out of the resonator, while the other waveguide is on Silica cantilever. Stressed arm experiences the strain during Protein (Biomolecules) adhesion. We analytical found refractive index change in accordance with applied strain as given by eq.5. The results of the simulations are +1.56 nm shift with -15000 με and -1.6 nm for +15000 με. The discrepancies between analytical and FDTD simulation results could be accounted as follows:

In eq.5, n and Δn are refractive index and change due to strain/stress respectively. In real scenario, one has to substitute effective index of the propagating mode. Dispersion effects in high index material such as SOI should be included in simulations. The FDTD simulator has taken these above mentioned factors into account and hence the results are different for both cases.

Conclusions

In this work, we designed and optimized an integrated optic sensor to monitor and measure conformation of proteins over a cantilever's surface. We designed the strip waveguide based racetrack resonator with radius of 3μm , and coupler length of 10μm that interrogates the cantilever movements. The cantilever is the extension of buffer layer of the SOI wafer, having a dimension of 100μm x 10μm x 1μm. Tensile and compressive strains of magnitude 15000 με are applied on the surface of cantilever beam and resonator's spectral characteristics are studied by analytical and numerical methods. FDTD simulations show that resonance wavelength experiences +1.56 nm shift with -15000 με and -1.6 nm for +15000 με strain. Our future work involves integration of optical and mechanical structures in suitable simulation domain.

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Sathish Malathi received her bachelor degree in Electronics and communication engineering from University of Madras, India in 1996 and masters degree in Microwave and optical engineering from Madurai Kamaraj University, India in 1999. She submitted her thesis for PhD degree in Electrical and communication engineering department, Indian Institute of Science, Bangalore, India under the supervision of Dr.T.Srinivas

She was working as a faculty in Adhiymaan College of engineering, Tamilnadu, India until December 2006. Her area of interest includes Integrated optic waveguide based devices, MOEMS sensors and Biophotonics.

Mrs.Malathi is student member of IEEE and SPIE. She is a life member of IETE (Institution of Electronics and Telecommunication Engineering)

Srinivas Talabatulla received his B.Sc (Hon) degree from Nehru science college, Hyderabad, India and PhD degree from Indian Institute of Science, Bangalore, India in 1992.

He was a Postdoctoral fellow at Toyohashi university of technology, Japan from 1992 to 1996. He is currently working as an Associate professor in Department of Electrical and Communication Engineering, Indian Institute of Science, India.

He is a member of IEEE Photonics and IEEE Comsoc.